LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135429.D
Acq On : 25 Sep 2023 16:19
Operator : CG\JU
Sample : 04540-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CENTRAL-M-R-HEATER

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135429.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.381	557	560	571	rBV	2186106	2271316	5.18%	2.918%
2	6.398	730	733	750	rVB	1367228	1482952	3.38%	1.905%
3	6.751	789	793	802	rVB	1249011	982434	2.24%	1.262%
4	7.322	881	890	893	rBV	3218363	3368901	7.68%	4.329%
5	8.028	1004	1010	1014	rBV	1354895	1307594	2.98%	1.680%
6	8.628	1107	1112	1115	rBV	3223093	3069263	7.00%	3.944%
7	9.110	1189	1194	1197	rBV	4987934	5007641	11.42%	6.434%
8	9.233	1210	1215	1221	rBV	494505	524912	1.20%	0.674%
9	9.516	1260	1263	1269	rBV	1024475	835348	1.90%	1.073%
10	9.786	1304	1309	1313	rBV2	1690950	1587496	3.62%	2.040%
11	10.110	1332	1364	1365	rBV3	6212402	43864491	100.00%	56.361%
12	10.592	1441	1446	1449	rBV	2786618	2830446	6.45%	3.637%
13	11.280	1559	1563	1567	rBV	1524405	1312469	2.99%	1.686%
14	11.822	1649	1655	1662	rVV	1249565	1639541	3.74%	2.107%
15	12.527	1770	1775	1783	rBV	304508	468164	1.07%	0.602%
16	12.610	1783	1789	1798	rVB	1064697	1411690	3.22%	1.814%
17	12.880	1830	1835	1838	rBV	3691695	3526867	8.04%	4.532%
18	13.939	2011	2015	2019	rVB	744674	704043	1.61%	0.905%
19	14.786	2155	2159	2167	rVB	670150	757007	1.73%	0.973%
20	15.404	2259	2264	2272	rVB	692358	875447	2.00%	1.125%

Sum of corrected areas: 77828022

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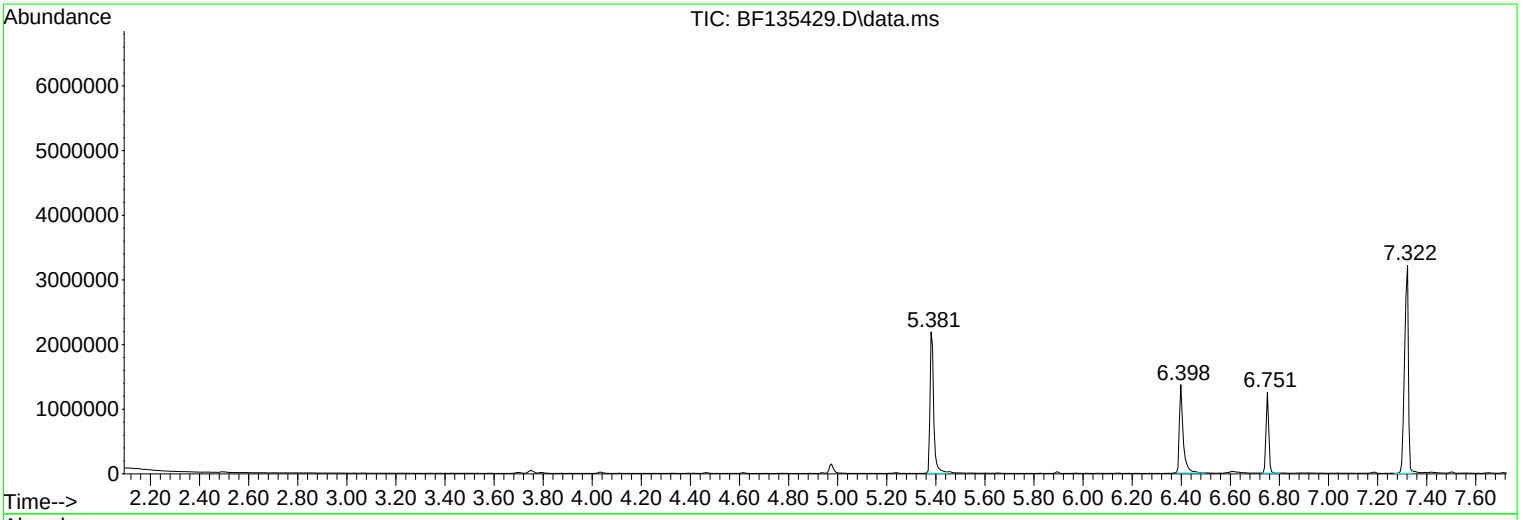
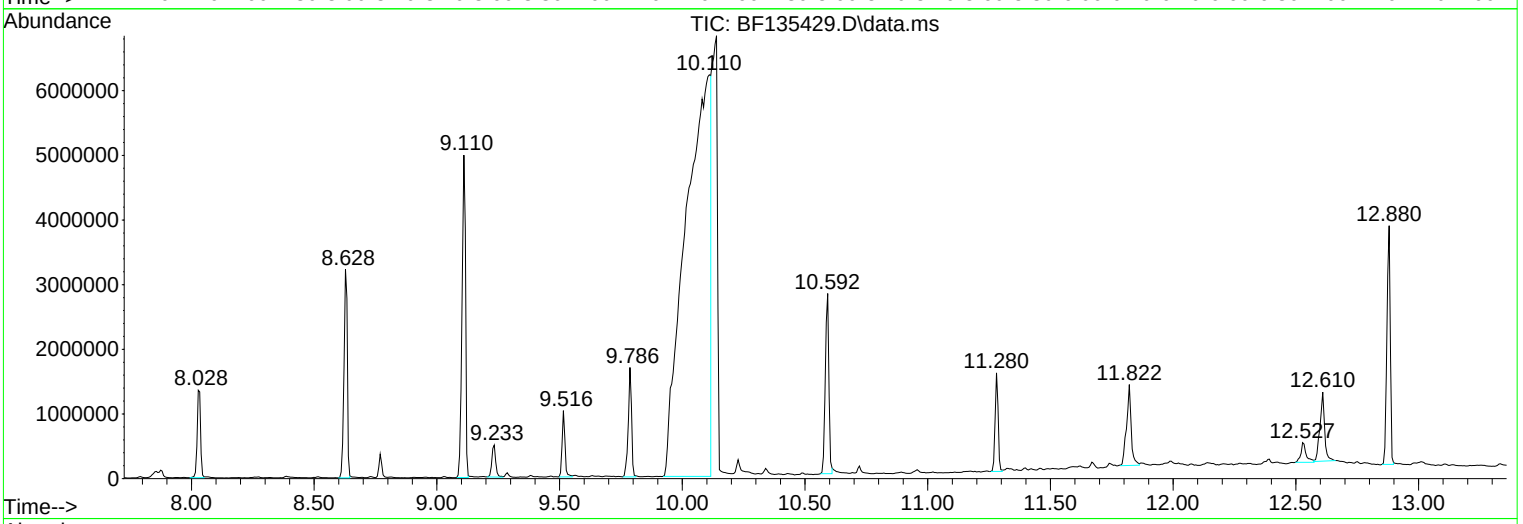
Misc :
ALS Vial : 10 Sample Multiplier: 1

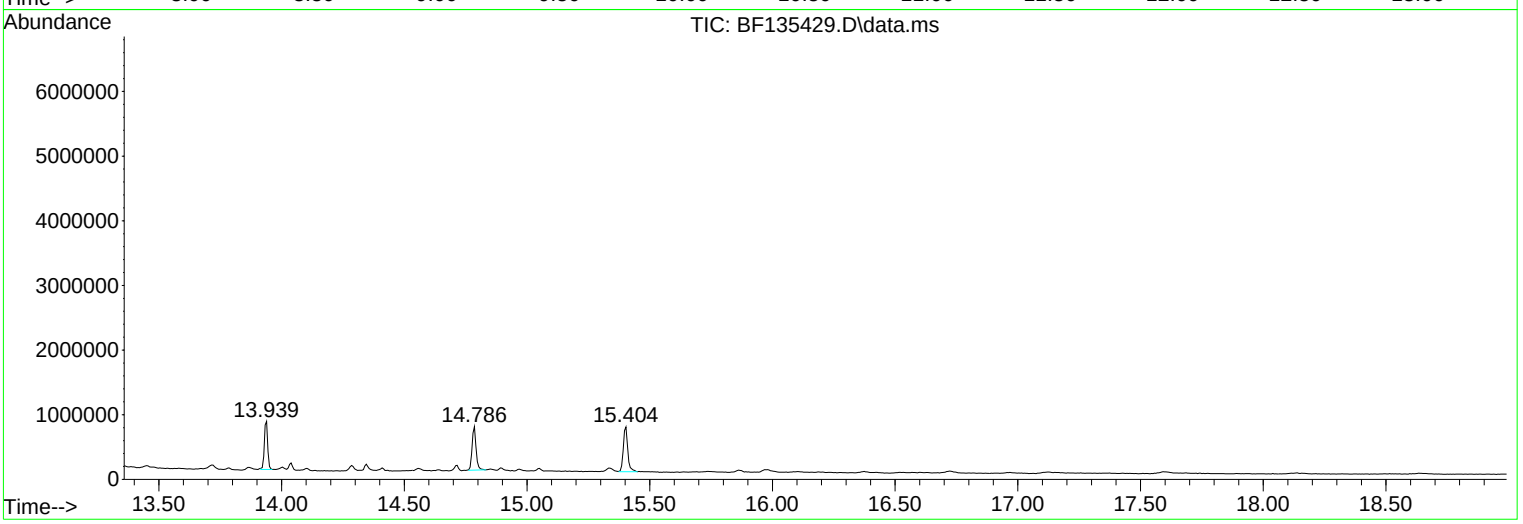
Instrument :
BNA_F
ClientSampleId :
CENTRAL-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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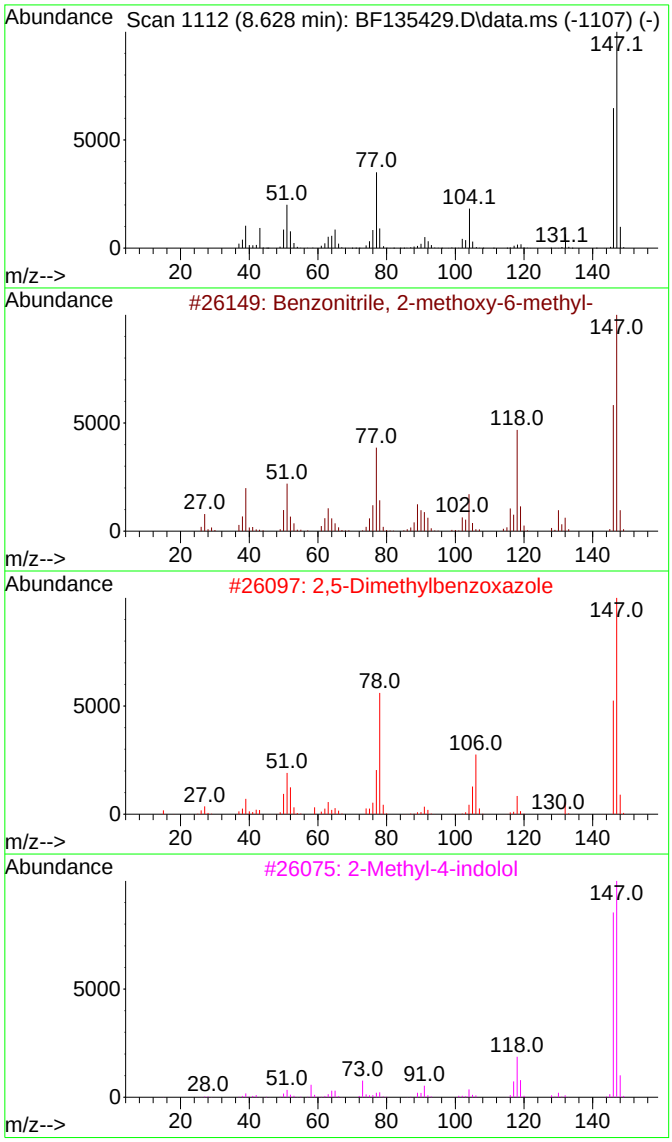
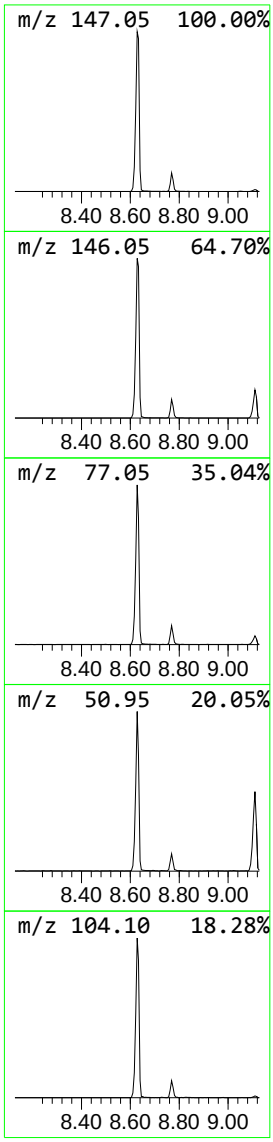
****

Peak Number 1 Benzonitrile, 2-methoxy-6-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	46.95 ng	3069260	Naphthalene-d8	8.034

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzonitrile, 2-methoxy-6-methyl-	147	C9H9NO	053005-44-0	86
2	2,5-Dimethylbenzoxazole	147	C9H9NO	005676-58-4	80
3	2-Methyl-4-indolol	147	C9H9NO	035320-67-3	50
4	(E)-N,N-Dimethyl-2-phenylethen-1...	147	C10H13N	1000482-46-2	47
5	(3-Methoxyphenyl)acetonitrile	147	C9H9NO	019924-43-7	47





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Misc :
ALS Vial : 10 Sample Multiplier: 1

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BNA_F
ClientSampleId :
CENTRAL-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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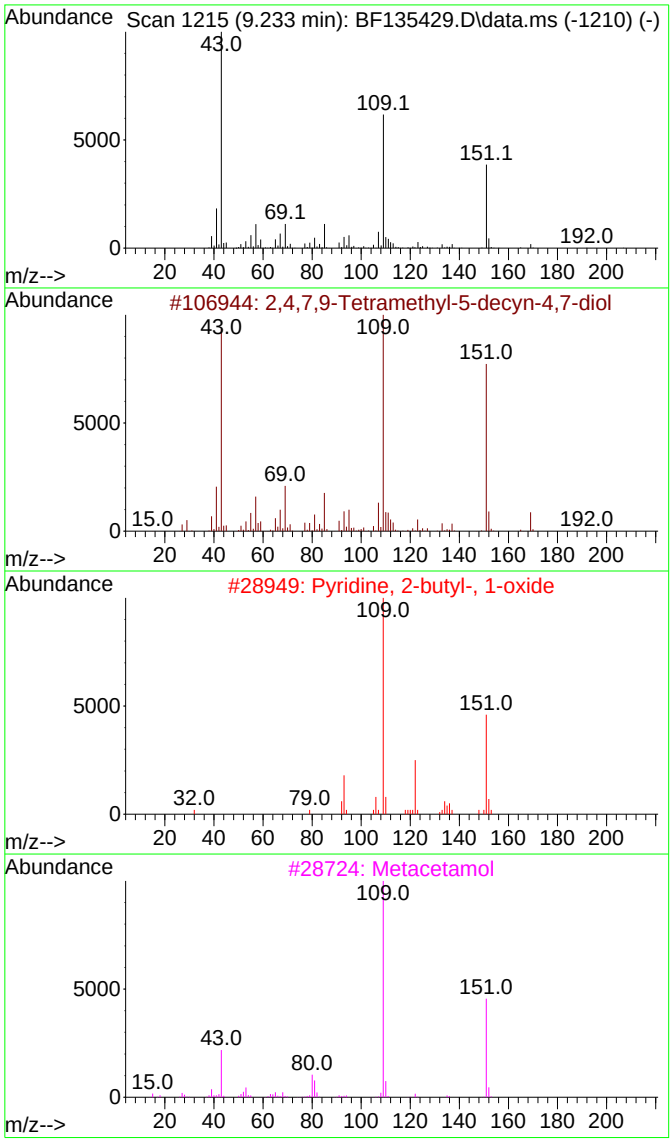
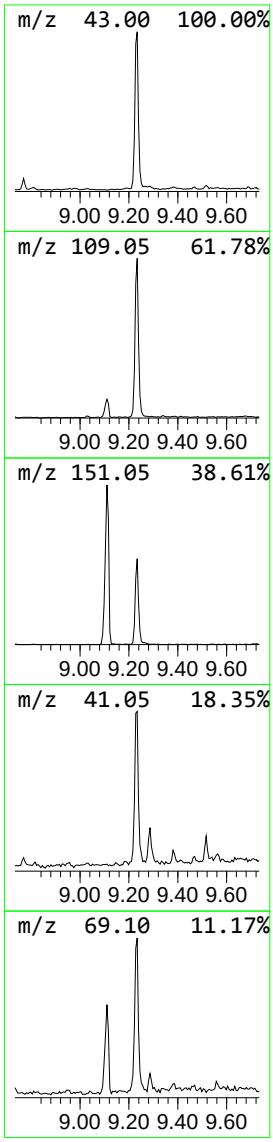
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.233	6.61 ng	524912	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	58
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	53
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53





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Instrument :
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ClientSampleId :
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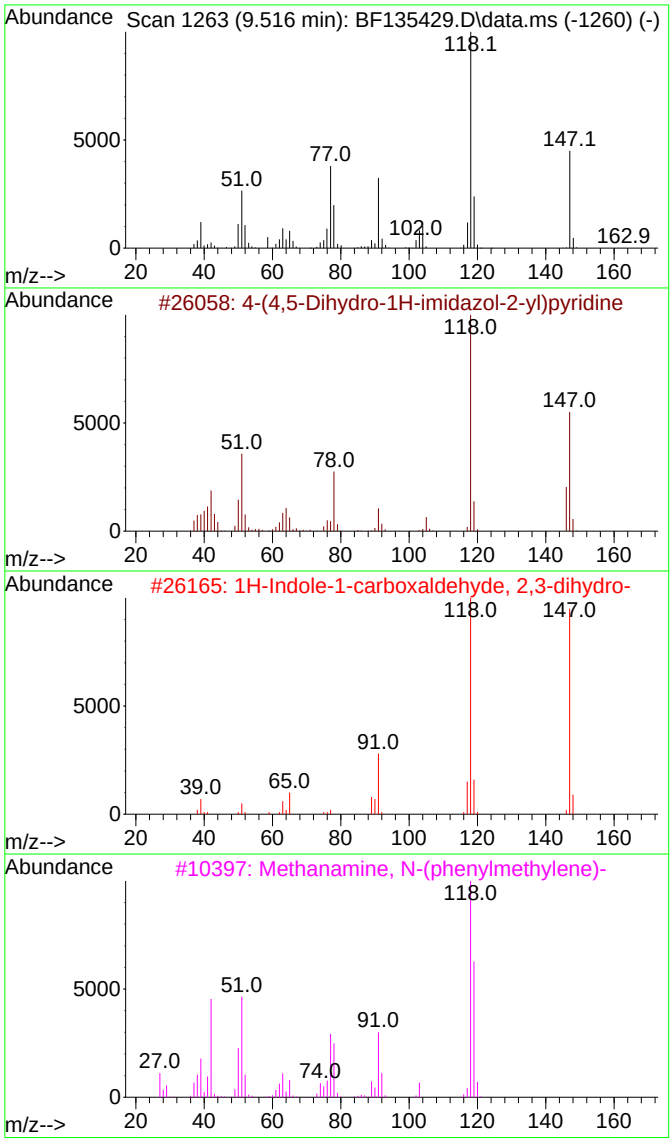
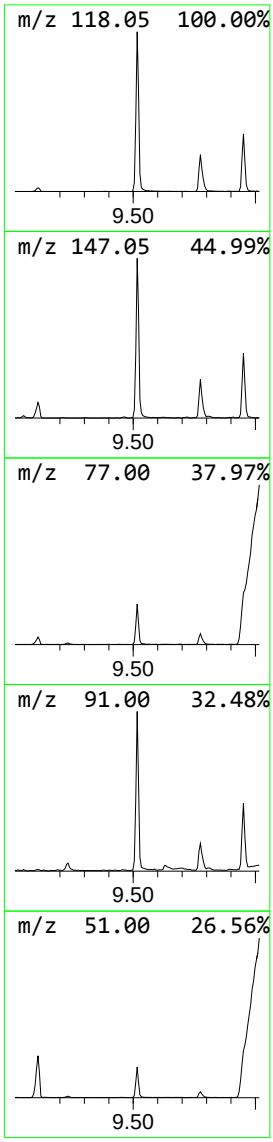
Peak Number 3 4-(4,5-Dihydro-1H-imidazol-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.516	10.52 ng	835348	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(4,5-Dihydro-1H-imidazol-2-yl)...	147	C8H9N3	021381-61-3	68
2	1H-Indole-1-carboxaldehyde, 2,3-...	147	C9H9NO	002861-59-8	50
3	Methanamine, N-(phenylmethylene)-	119	C8H9N	000622-29-7	43
4	3-(4,5-Dihydro-1H-imidazol-2-yl)...	147	C8H9N3	006302-53-0	42
5	2-Pyridylacetonitrile	118	C7H6N2	002739-97-1	35





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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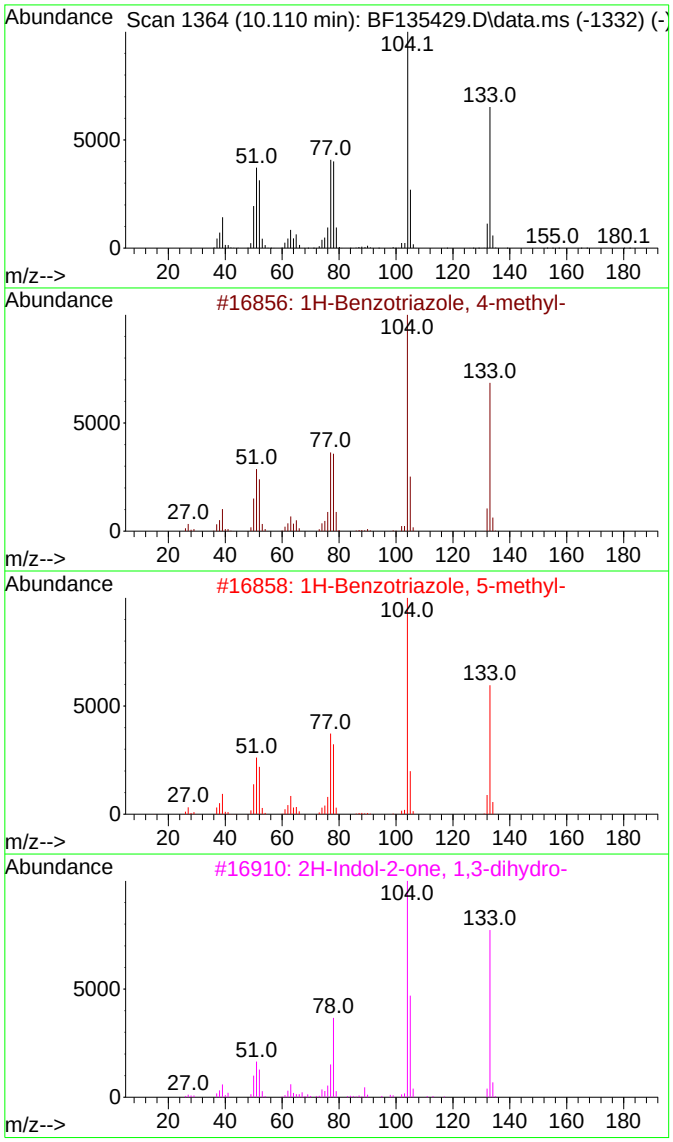
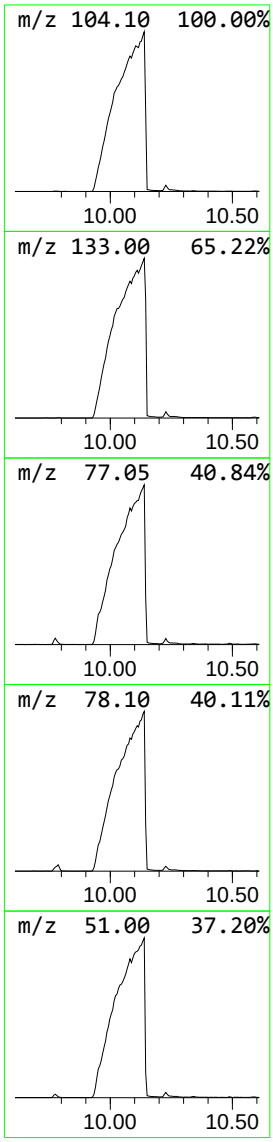
Peak Number 4 1H-Benzotriazole, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.110	552.63 ng	43864500	Acenaphthene-d10	9.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
3	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	80
4	1H-Indol-4-ol	133	C8H7NO	002380-94-1	49
5	Indan, epoxide	132	C9H8O	000768-22-9	47





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CENTRAL-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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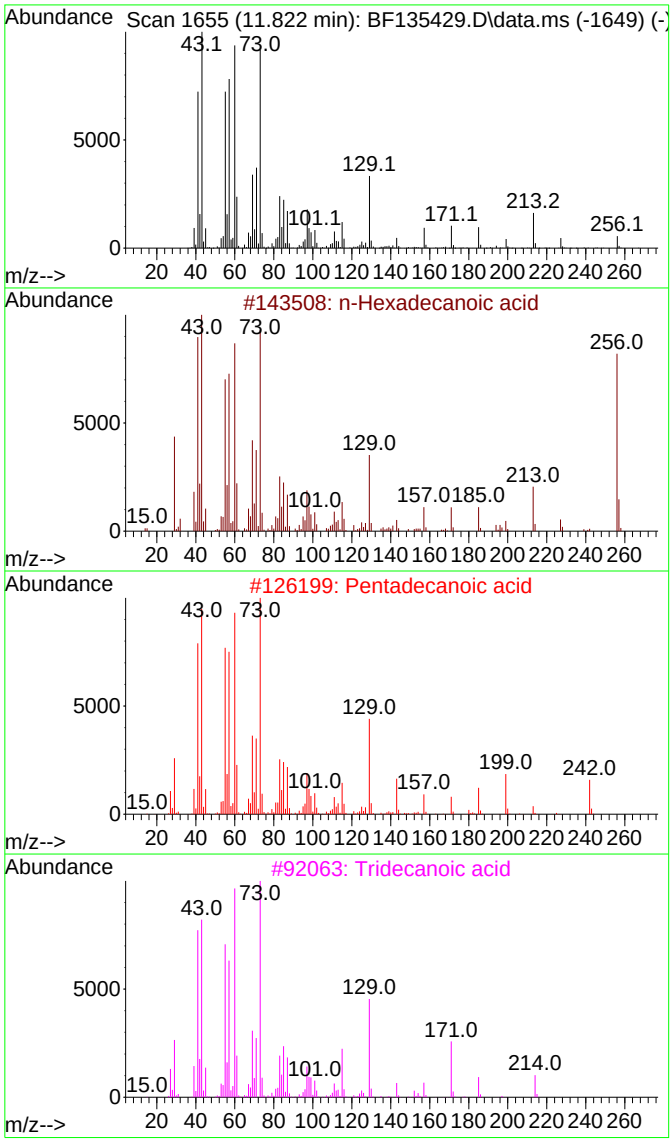
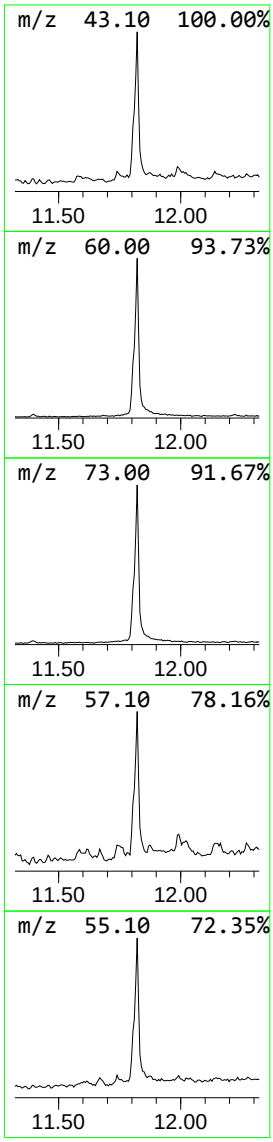
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	24.98 ng	1639540	Phenanthrene-d10	11.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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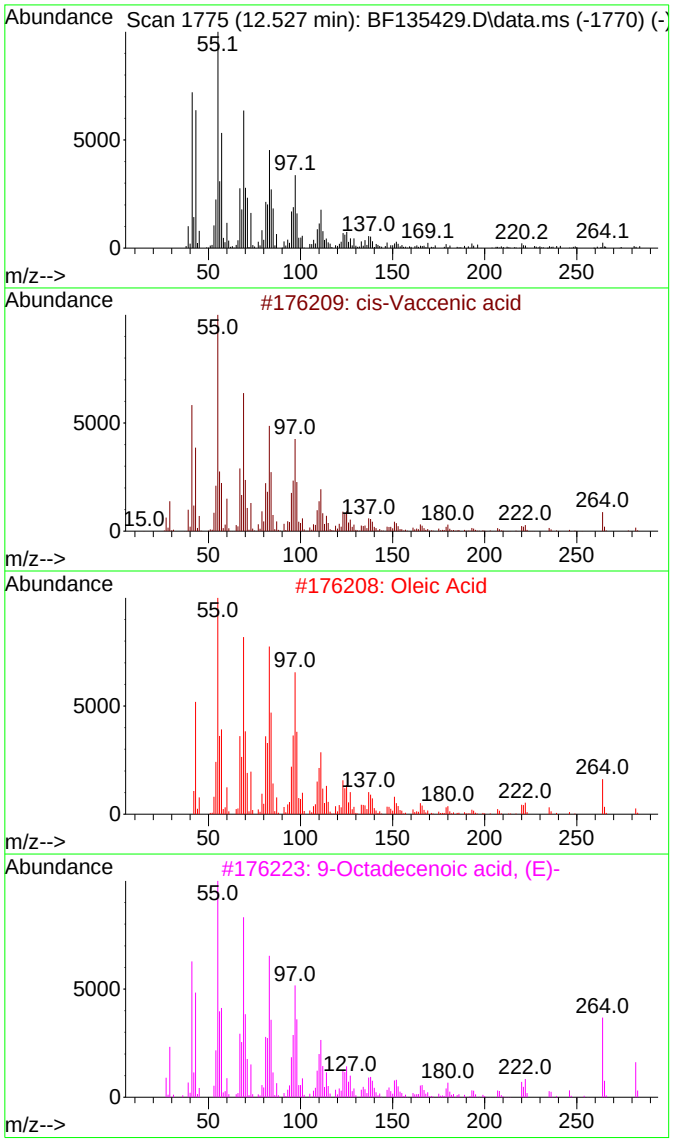
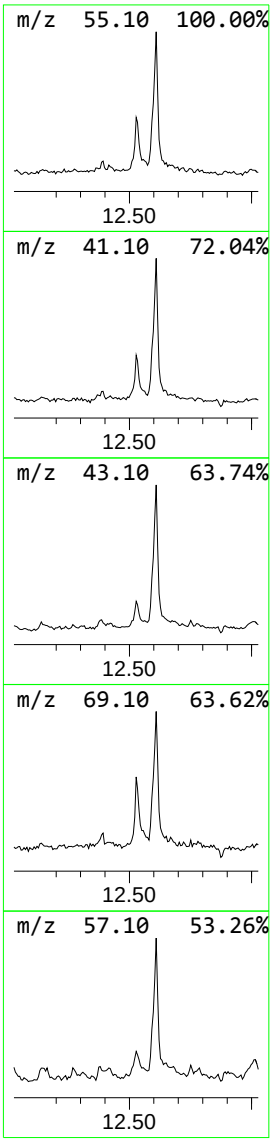
****

Peak Number 6 cis-Vaccenic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	7.13 ng	468164	Phenanthrene-d10	11.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2	Oleic Acid	282	C18H34O2	000112-80-1	96
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	90
5	9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	90





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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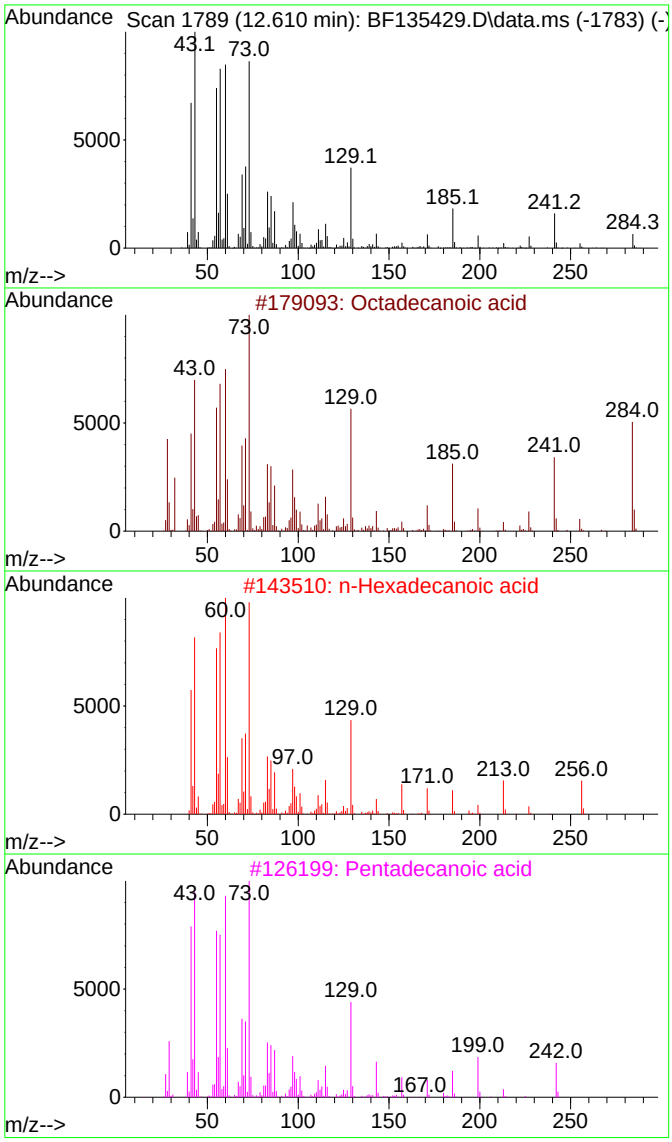
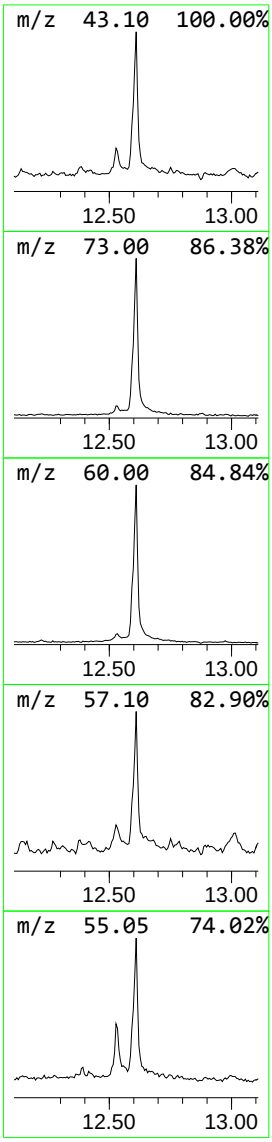
****

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	40.10 ng	1411690	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





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TIC Library : C:\Database\NIST20.L
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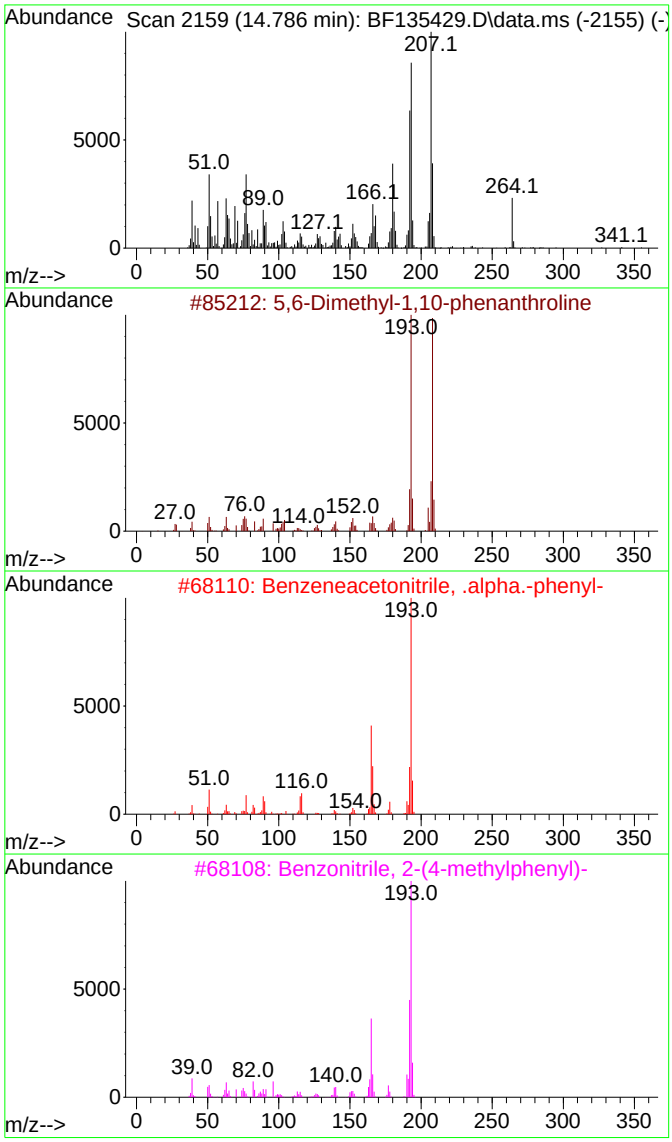
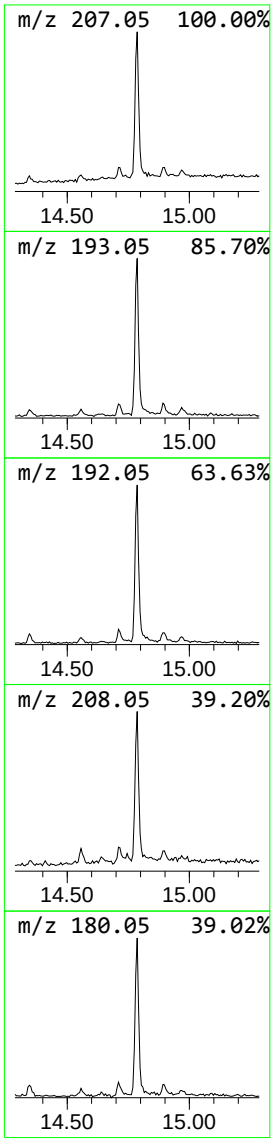
Peak Number 8 unknown14.786 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	17.29 ng	757007	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6-Dimethyl-1,10-phenanthroline	208	C14H12N2	003002-81-1	41
2	Benzeneacetonitrile, .alpha.-phe...	193	C14H11N	000086-29-3	38
3	Benzonitrile, 2-(4-methylphenyl)-	193	C14H11N	114772-53-1	30
4	4',6'-Dimethoxy-2',3'-dimethylac...	208	C12H16O3	1010244-80-3	25
5	9-Vinylcarbazole	193	C14H11N	001484-13-5	25





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzonitrile, 2...	8.628	47.0	ng	3069260	2	8.034	1307590	20.0
2,4,7,9-Tetrame...	9.233	6.6	ng	524912	3	9.786	1587500	20.0
4-(4,5-Dihydro-...	9.516	10.5	ng	835348	3	9.786	1587500	20.0
1H-Benzotriazol...	10.110	552.6	ng	43864500	3	9.786	1587500	20.0
n-Hexadecanoic ...	11.822	25.0	ng	1639540	4	11.280	1312470	20.0
cis-Vaccenic acid	12.527	7.1	ng	468164	4	11.280	1312470	20.0
Octadecanoic acid	12.610	40.1	ng	1411690	5	13.939	704043	20.0
unknown14.786	14.786	17.3	ng	757007	6	15.404	875447	20.0